

Characterization of yak common biofluids metabolome by means of proton nuclear magnetic resonance spectroscopy

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SUPPLEMENTAL MATERIAL

Table S1: Metabolites identified by ¹H-NMR in yak biofluids.

Molecules	ppm	Functional group	Multiplicity	Molecule source	Groups
1,3-Dihydroxyacetone	4.4122	CH ₂	s	D	Serum
2,6-Dihydroxybenzoate	6.4221	CH-2	d	D	Urine
2-Aminobutyrate	0.9648	CH ₃	t	P	Serum
2-Hydroxy-3-methylvalerate	0.9310	CH ₃ -9	d	P	Urine
2-Hydroxybutyrate	0.8859	CH ₃	t	P	Serum
2-Hydroxyisobutyrate	1.3478	CH ₃	s	D	Urine
2-Hydroxyisovalerate	0.8244	CH ₃	d	P	Urine
2-Hydroxyvalerate	0.8970	CH ₃	t	E	Urine
2-Oxoisocaproate	2.6038	CH ₂	d	P	Feces
3-Hydroxybutyrate	1.1863	CH ₃	d	E	Serum, Urine, Feces
3-Hydroxyisobutyrate	1.0503	CH ₃	d	P	Serum, Urine
3-Hydroxyisovalerate	1.2585	CH ₃	s	P	Urine
3-Hydroxyphenylacetate	3.4718	CH ₂	s	P	Urine
3-Indoxylsulfate	7.6894	CH-6	d	D, P	Urine
3-Methyl-2-oxovalerate	1.1042	CH ₃ -9	d	P	Urine
3-Methylglutarate	0.9095	CH ₃	d	P	Urine
3-Methylhistidine	7.1366	CH-5	s	P	Serum
3-Phenylpropionate	2.8659	CH ₂ -7	m	p	Urine, Feces
4-Hydroxyphenylacetate	6.8582	CH-3	d	D	Urine, Feces
Acetate	1.9071	CH ₃	s	P	Serum, Urine, Feces
Acetoacetate	2.2688	CH ₃	s	E	Serum, Feces
Acetoin	1.3583	CH ₃ -3	d	E	Feces
Acetone	2.2178	CH ₃	s	E	Serum, Feces
Adenosine	8.3436	CH-7	s	P	Urine
Alanine	1.4675	CH ₃	d	P	Serum, Urine, Feces
Allantoin	5.3643	CH	s	P, M	Urine
Arabinose	4.5038	CH-2	d	M, E	Serum
Arginine	1.9229	CH ₂ -6	m	P	Serum

Ascorbate	4.5072	CH	d	D, E	Urine
Asparagine	2.9282	CH ₂	dd	P	Serum
Aspartate	2.7842	CH ₂	dd	P	Serum, Feces
<i>beta</i> -Alanine	2.5558	CH ₂ -4	t	P	Serum, Urine
Betaine	3.8894	CH ₂	s	P	Serum, Urine
Butyrate	0.8818	CH ₃	t	E	Feces
Carnitine	3.2208	CH ₃	s	E	Serum, Feces
Choline	3.1888	CH ₃	s	E, P	Serum, Feces
<i>cis</i> -Aconitate	3.1089	CH ₂	d	E	Urine
Citrate	2.5093	CH ₂	d	P	Serum, Urine
Creatine	3.0222	CH ₂	s	P	Serum, Urine, Feces
Creatinine	3.0325	CH ₃	s	P	Serum, Urine
Dimethyl sulfone	3.1391	CH ₃	s	D, M	Serum, Urine, Feces
Dimethylamine	2.7117	CH ₃	s	P	Serum, Urine
Dimethylglycine	2.9124	CH ₃	s	E, P	Serum, Urine
Ethanol	1.1699	CH ₃	t	E, M	Serum, Urine, Feces
Ethylmalonate	1.7091	CH ₂	m	E	Urine
Formate	8.4446	CH	s	E	Serum, Urine, Feces
Fucose	1.2024	CH ₃	d	E	Urine, Feces
Fumarate	6.5090	CH-5	s	E	Serum, Feces
Galactarate	4.2597	CH	s	E	Urine
Galactose	4.5825	CH-2	d	E	Feces
Gluconate	4.1362	CH-9	d	E	Urine
Glucose	3.2233	CH-2	dd	D, E	Serum, Urine, Feces
Glutamate	2.0606	CH ₂ -6	m	P	Serum, Feces
Glutamine	2.4430	CH	m	P	Serum, Urine
Glutarate	2.1540	CH ₂	t	E, P	Urine, Feces
Glycerol	3.5664	CH ₂	dd	E	Serum, Feces
Glycine	3.5533	CH ₂	s	P	Serum, Urine, Feces
Guanidoacetate	3.7782	CH ₂	s	P	Urine
Guanosine	5.8929	CH-2	d	P	Urine
Hippurate	3.9607	CH ₂	d	P	Urine
Isobutyrate	1.0473	CH ₃	d	M	Urine, Feces
Isocaproate	1.4133	CH ₂ -5	m	E	Urine
Isoleucine	1.0020	CH ₃ -9	d	P	Serum, Urine, Feces
Isovalerate	0.9030	CH ₃	d	P	Feces
Lactate	4.1059	CH	dd	E	Serum, Urine, Feces
Leucine	0.9356	CH ₃ -9	d	P	Serum, Feces
Lysine	3.0077	CH ₂ -9	t	P	Serum
Malonate	3.1199	CH ₂	s	D, E	Urine
Mannose	5.1767	CH-6	d	E	Serum
Methanol	3.3481	CH ₃	s	E	Serum, Urine, Feces
Methionine	2.6178	CH ₂ -3	t	P	Serum, Feces

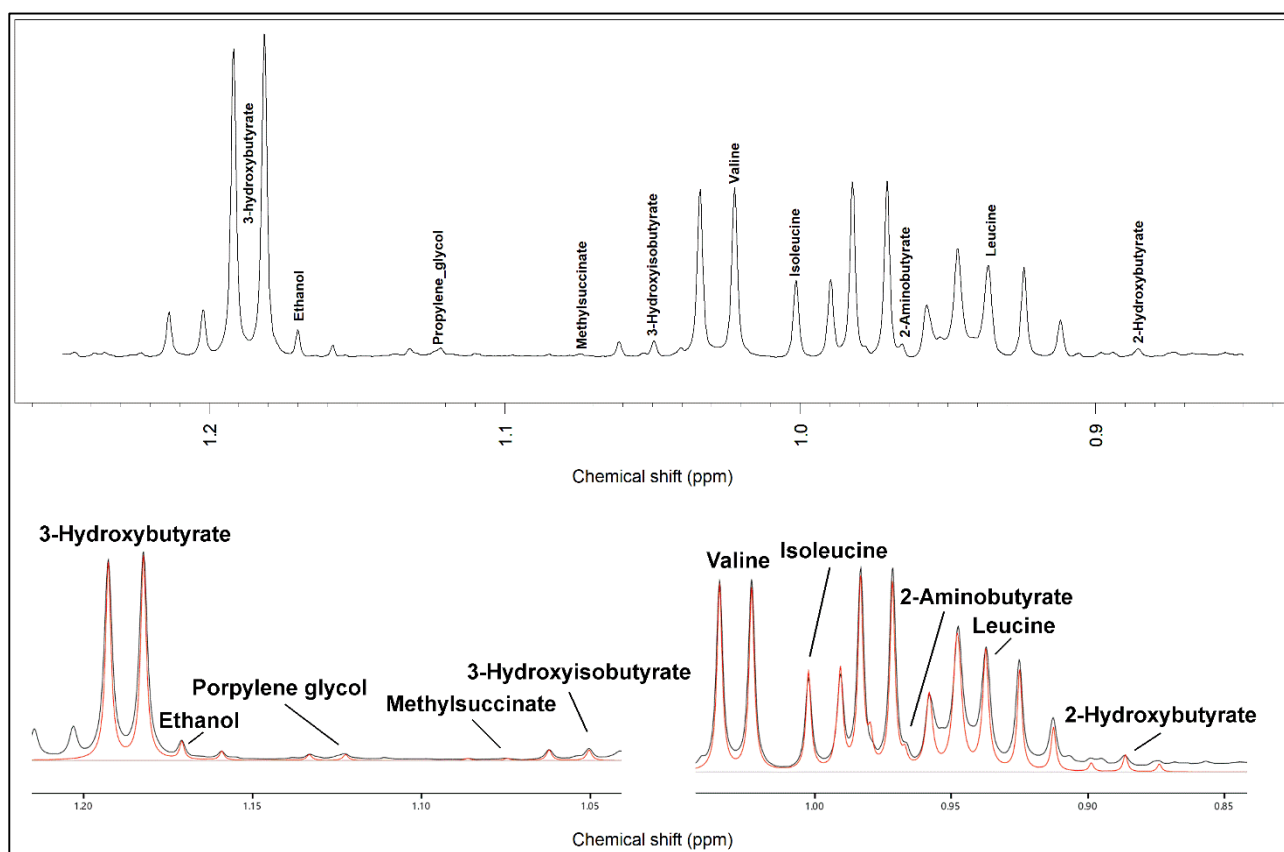
Methylamine	2.5878	CH ₃	s	D	Urine, Feces
Methylsuccinate	1.0742	CH ₃	d	P, E	Serum, Urine
myo-Inositol	4.0585	CH-2	t	E	Serum, Urine
N-Acetylglucosamine	5.1989	CH	d	E, P	Feces
N-Carbamoylaspartate	2.6698	CH ₂	dd	P	Serum
N-Methylhydantoin	2.9129	CH ₃	s	P	Feces
N-Phenylacetyl glycine	3.6605	CH ₂ -11	s	P	Urine, Feces
O-Acetylcholine	3.2081	CH ₃	s	E	Feces
O-Phosphocholine	3.1977	CH ₃	s	E	Feces
Ornithine	3.0440	CH ₂ -8	t	P	Serum
<i>p</i> -Cresol	6.8170	CH-2	d	P	Urine
Phenylacetate	7.2826	CH-4	m	P	Feces
Phenylalanine	7.3669	CH-4	t	P	Serum, Feces
Proline	1.9998	CH ₂ -3	m	P	Serum
Propionate	1.0292	CH ₃	t	P	Feces
Propylene glycol	1.1227	CH ₃	d	E	Serum, Urine
Pyruvate	2.3573	CH ₃	s	E	Serum, Urine
Sarcosine	2.7262	CH ₃	s	P	Serum, Urine
Serine	3.9555	CH ₂	dd	P	Serum, Feces
Serotonin	3.3023	CH ₂	t	P	Urine
Succinate	2.3933	CH ₂	s	P, E	Serum, Urine, Feces
Tartrate	4.3311	CH	s	D	Urine
Taurine	3.2368	CH ₂ -6	t	P	Urine
Threonine	3.5838	CH-4	d	P	Serum, Feces
Tiglylglycine	6.4968	CH	m	P	Urine
<i>trans</i> -Aconitate	6.5814	CH	s	E	Urine
Trehalose	5.1837	CH	s	E	Feces
Trigonelline	4.4165	CH ₃	s	D	Urine
Trimethylamine	2.8226	CH ₃	s	D	Serum, Urine
Trimethylamine N-oxide	3.2589	CH ₃	s	D	Urine
Tyrosine	7.1776	CH-3	d	P	Serum, Urine, Feces
Uracil	5.7903	CH-5	d	P	Serum, Feces
Uridine	5.9079	CH-2	d	P	Serum
Valerate	0.8756	CH ₃	t	D	Feces
Valine	1.0206	CH ₃ -7	d	P	Serum, Urine, Feces
Xanthosine	5.8460	CH-2	d	P	Urine
Xylose	4.5781	CH-2	d	E	Urine

Molecules assignment and quantification

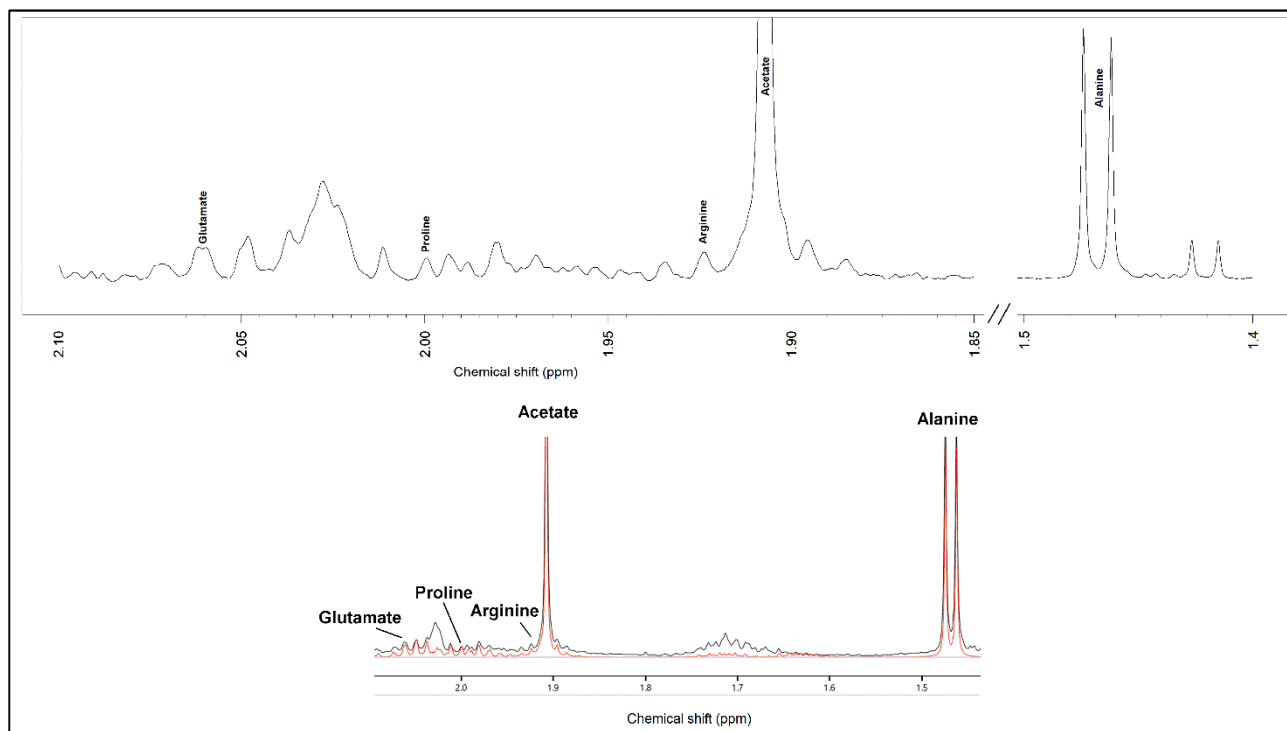
Figures S1-S36: Pictorial description of the molecules assignment procedure by Chenomx software. Upper panel - portions of the representative spectrum. Lower panel - The spectrum (black line) superimposed to the simulated signals (red line) for each of the molecules listed. The line connecting each name with the spectra highlights the signal used for quantification purposes.

Yak Serum

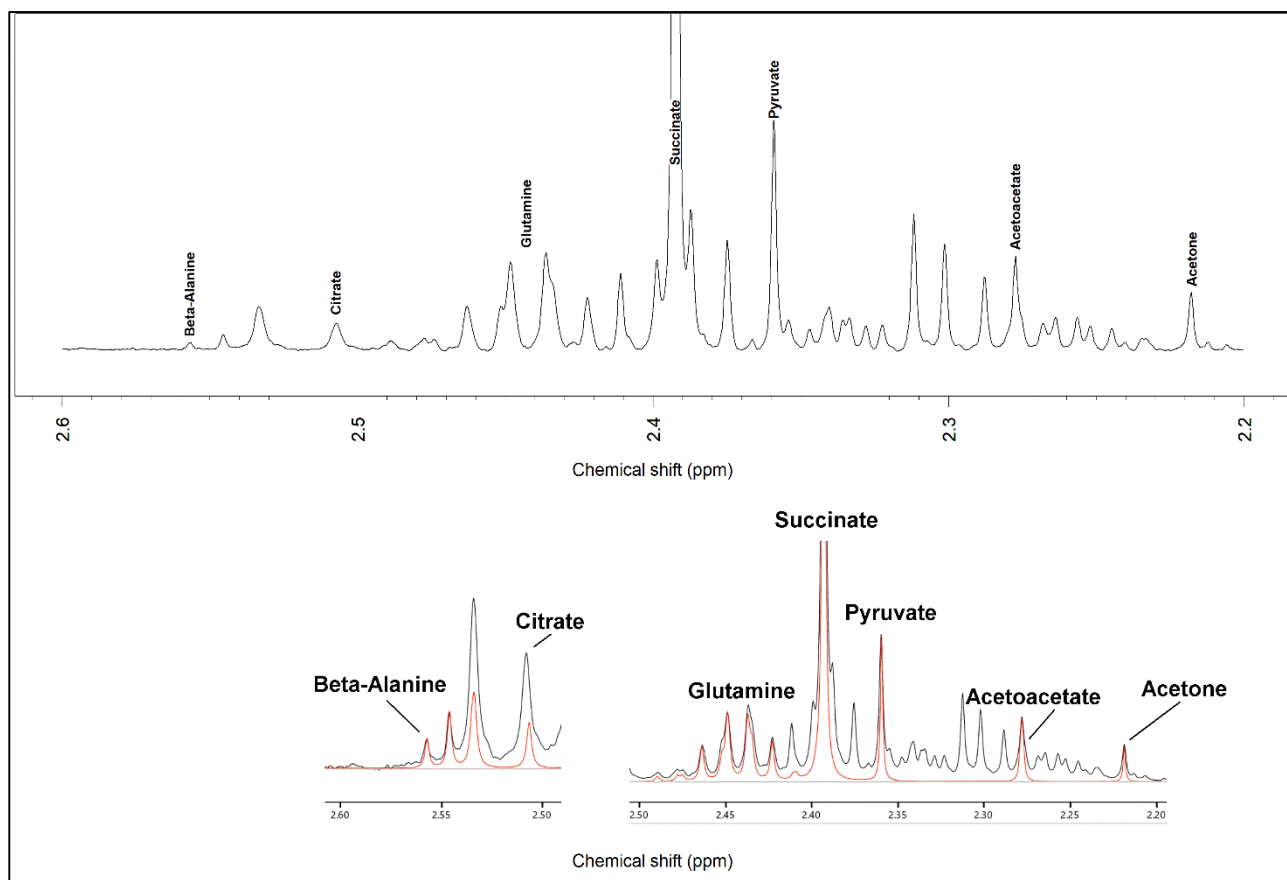
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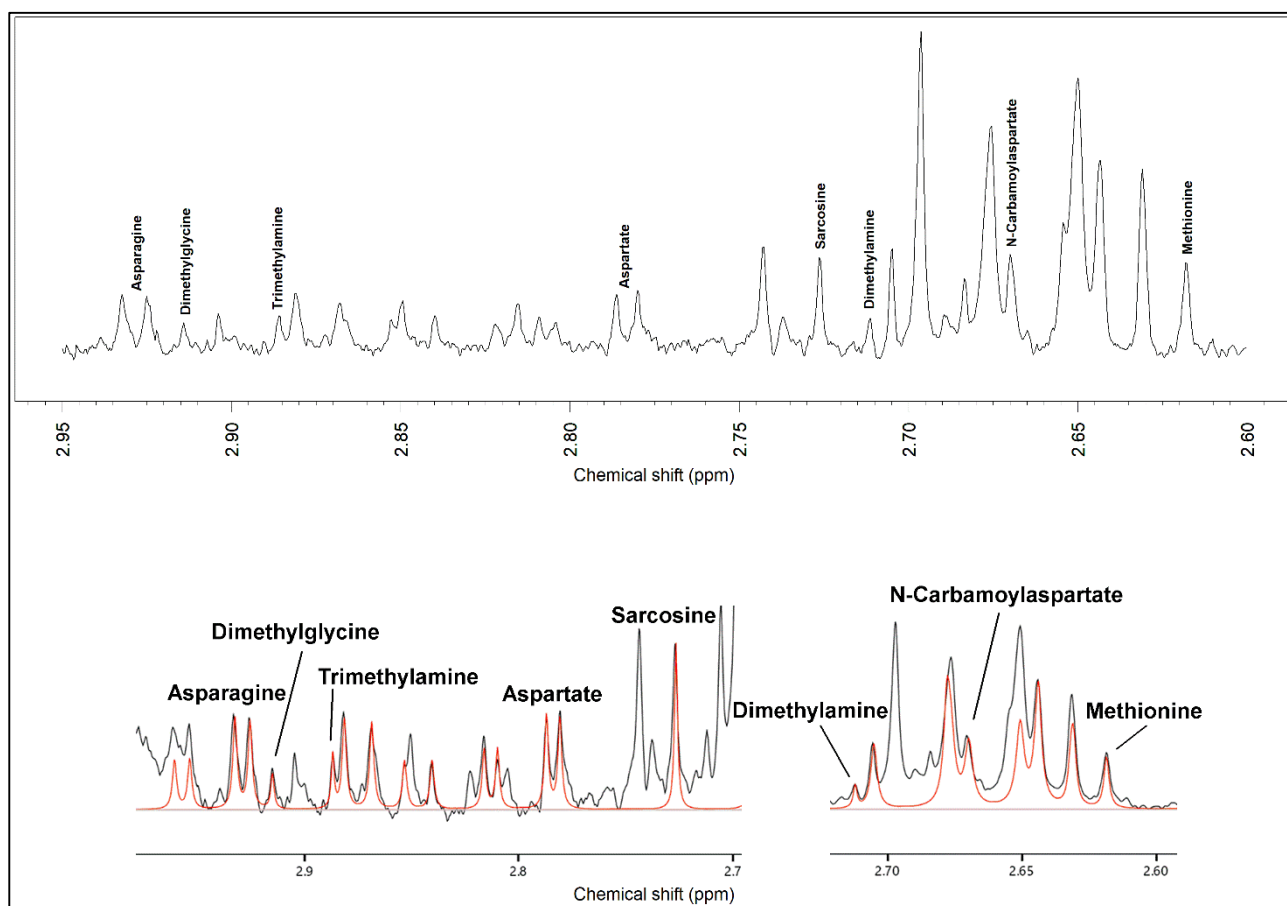
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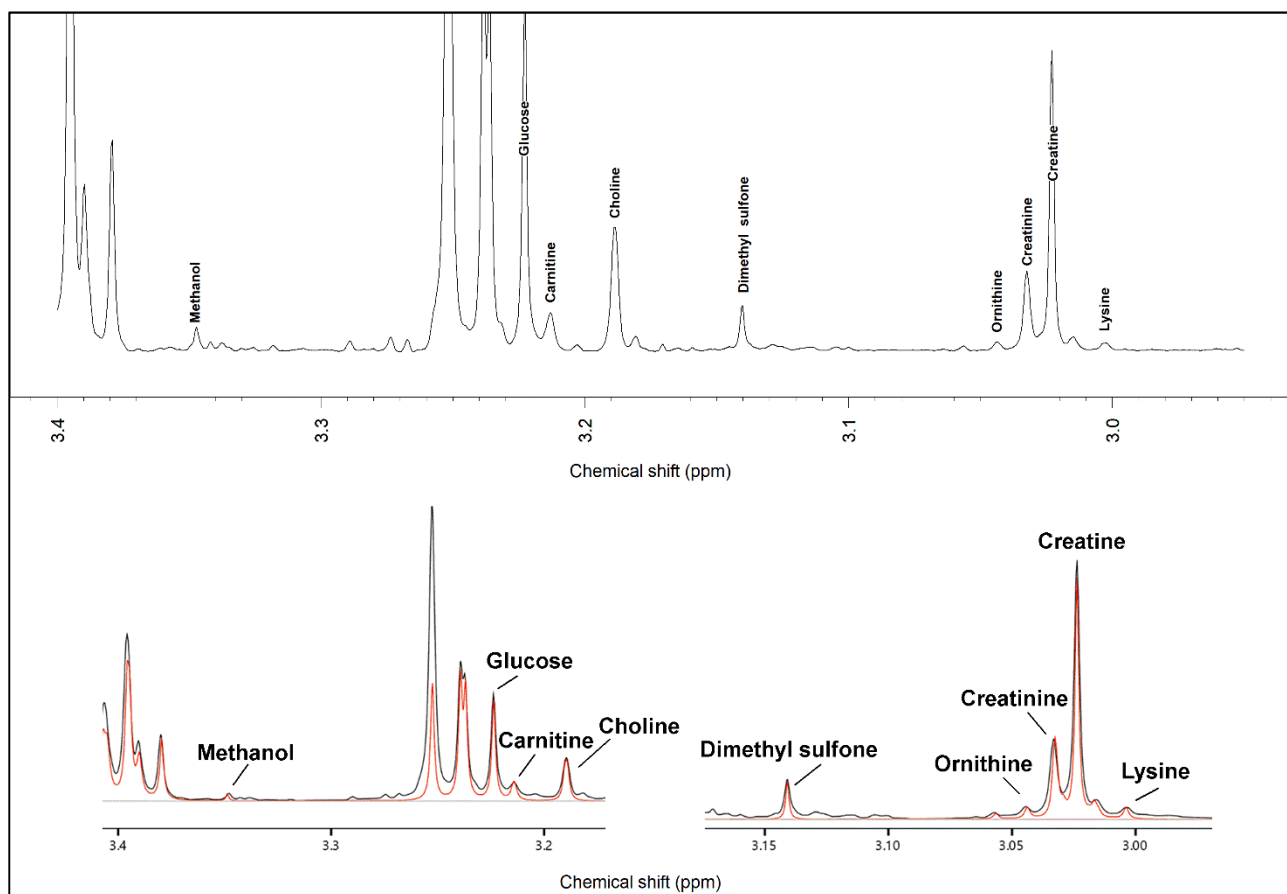
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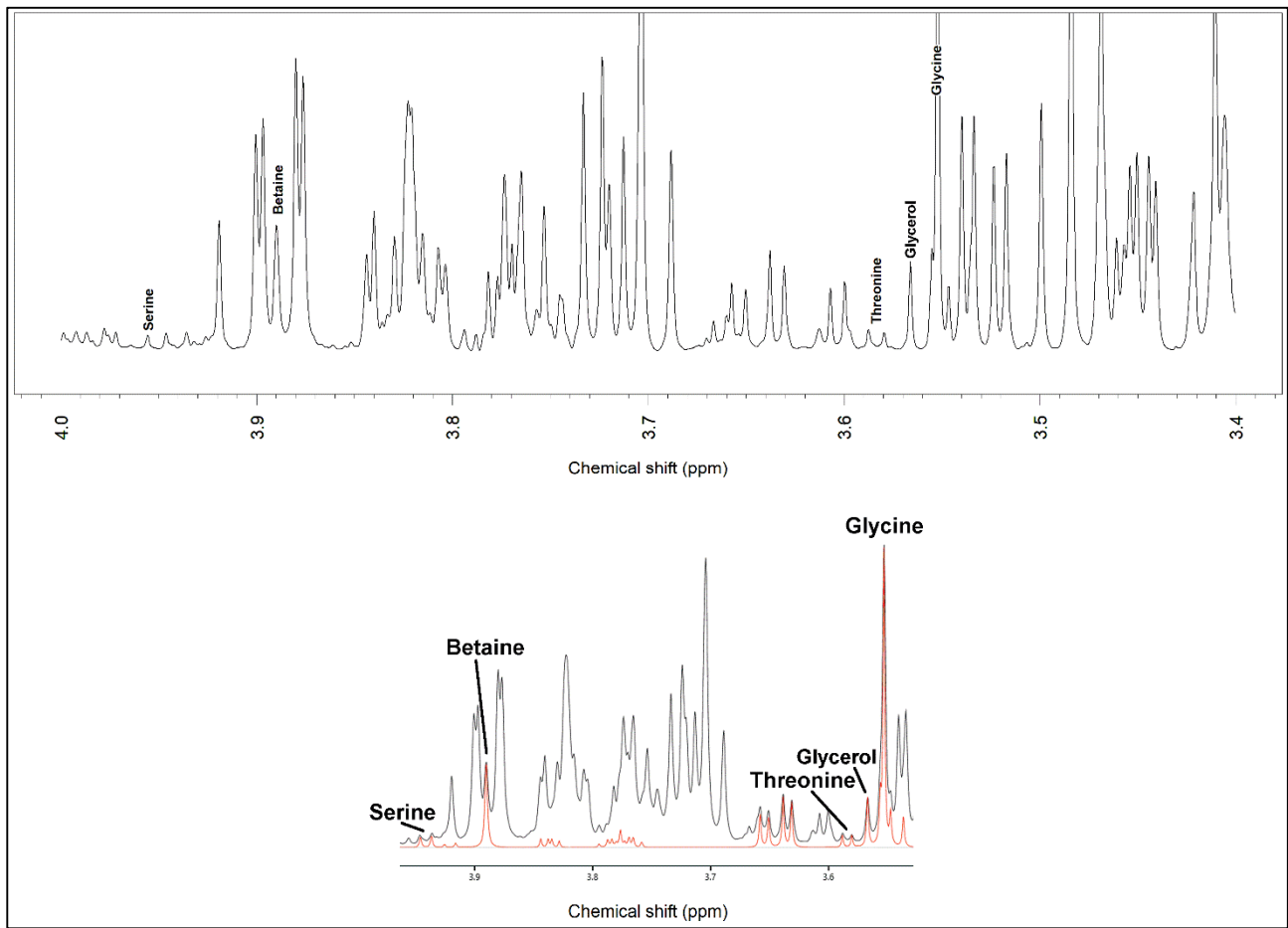
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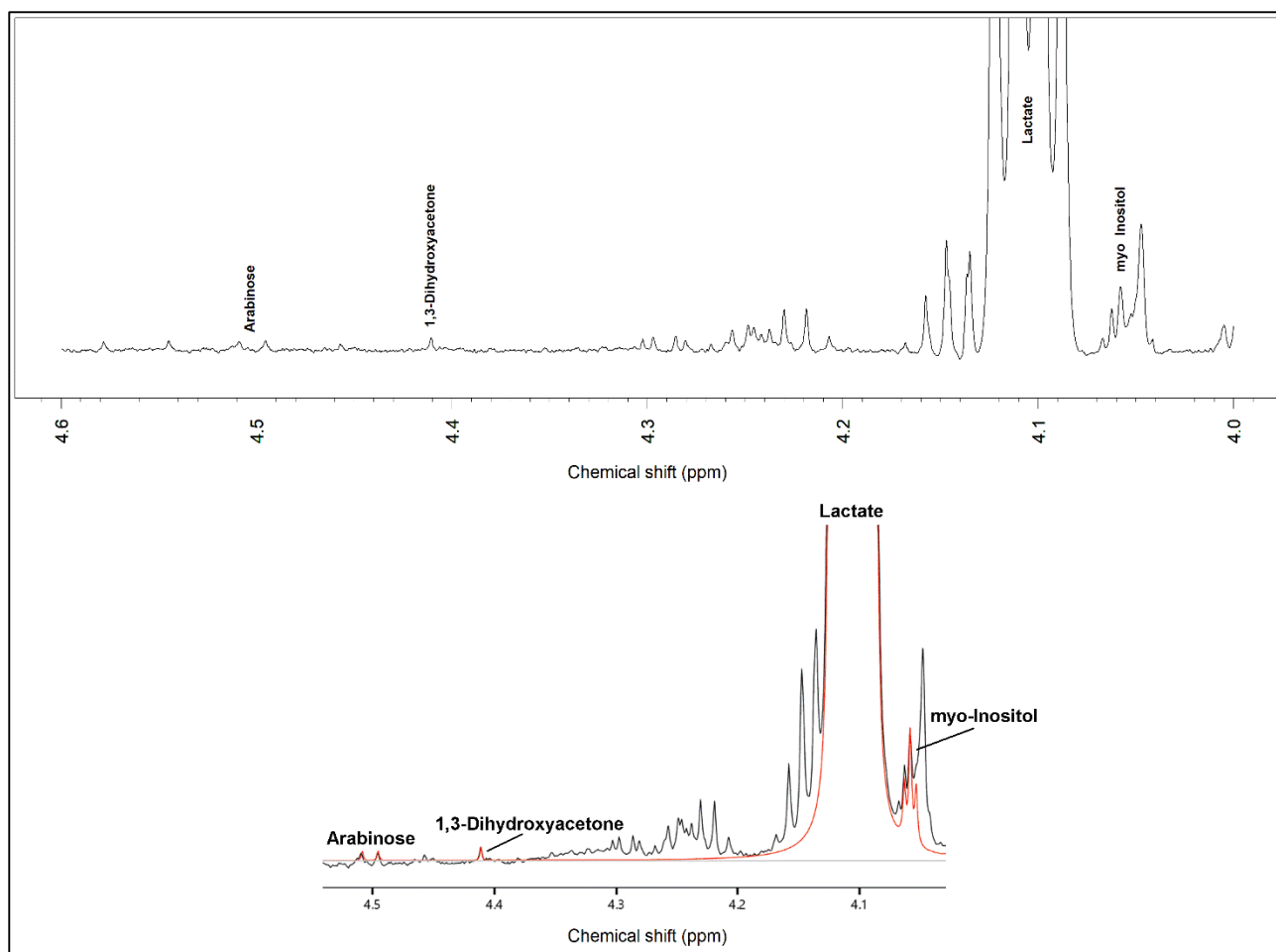
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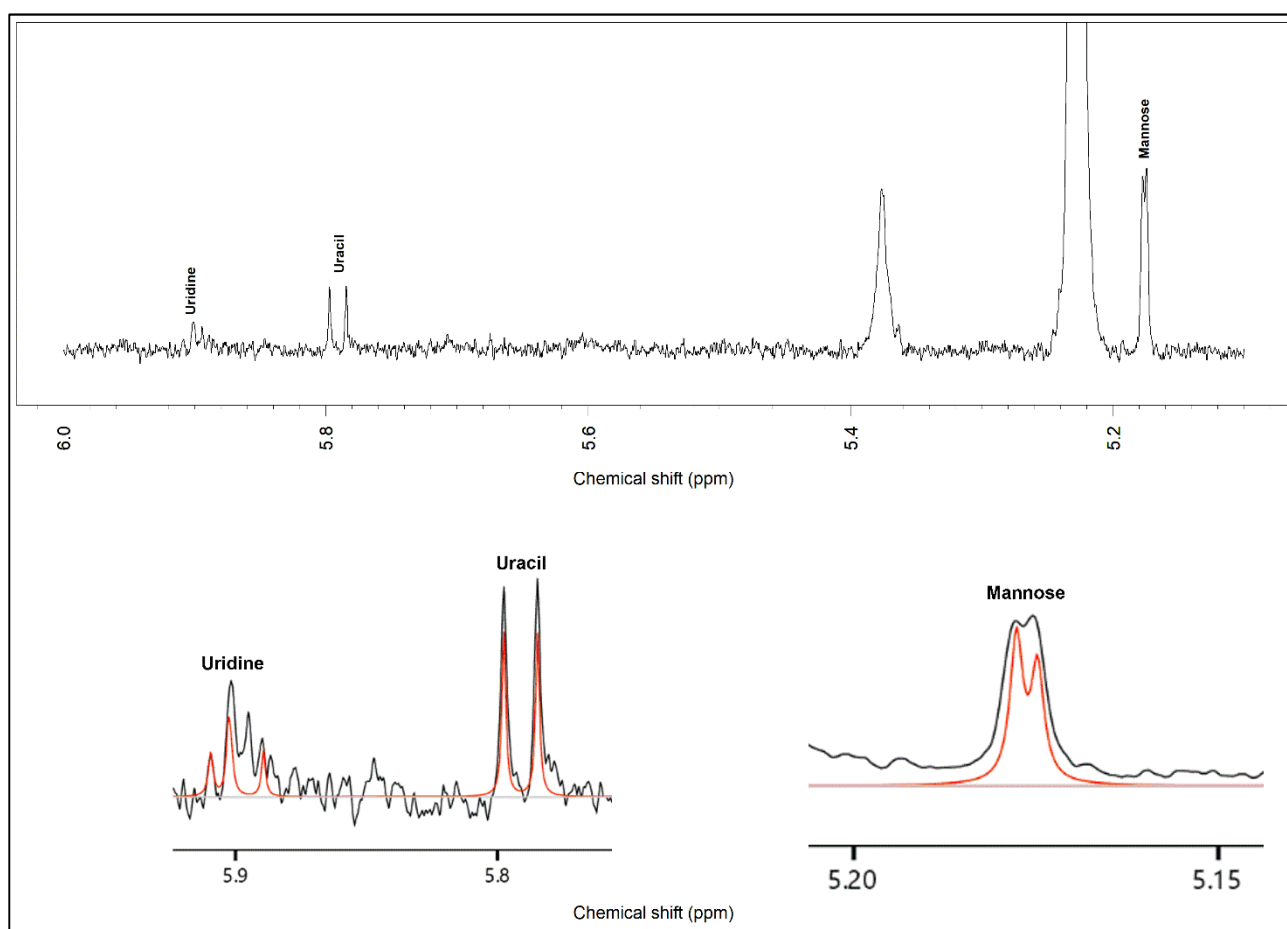


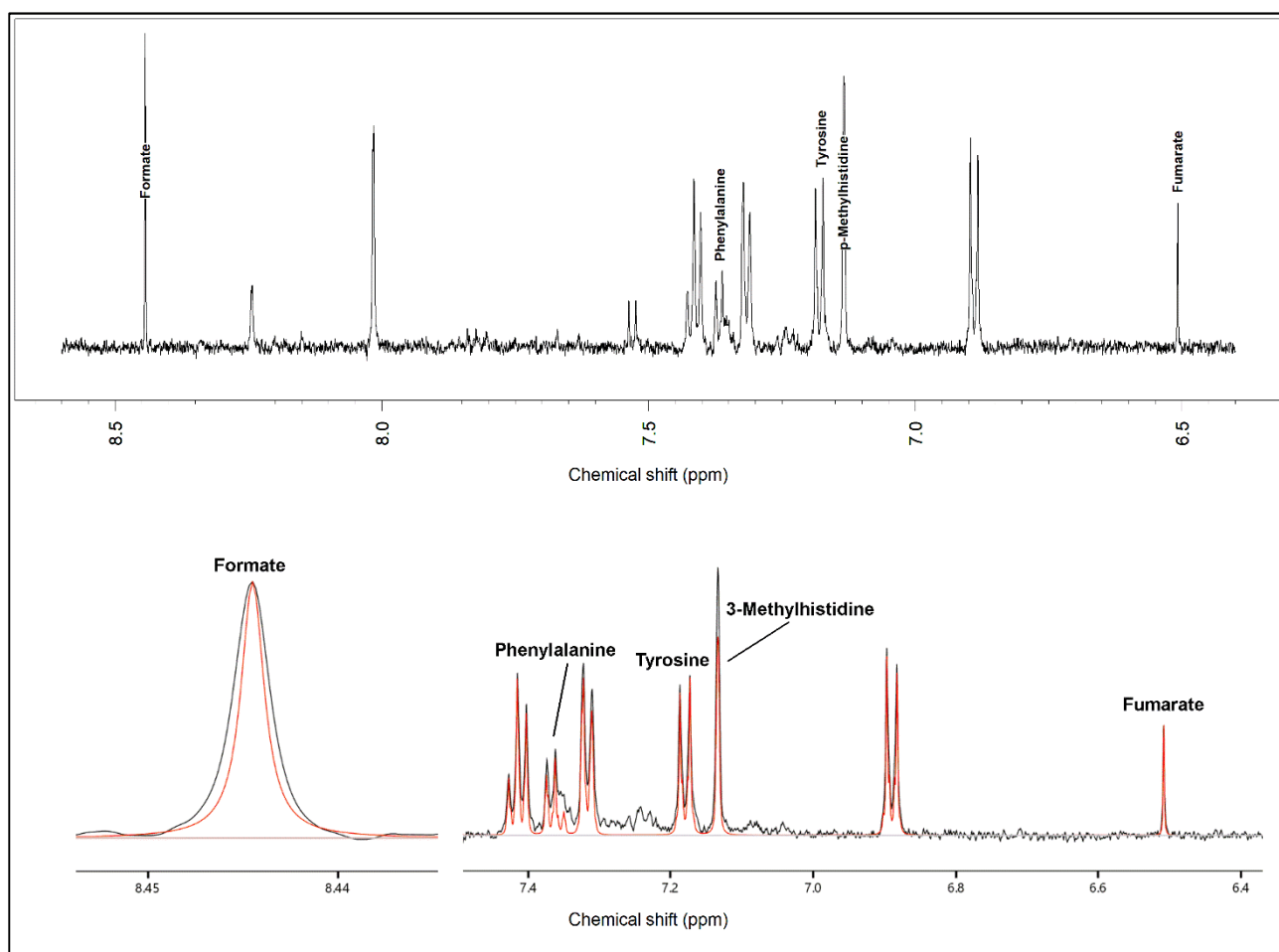
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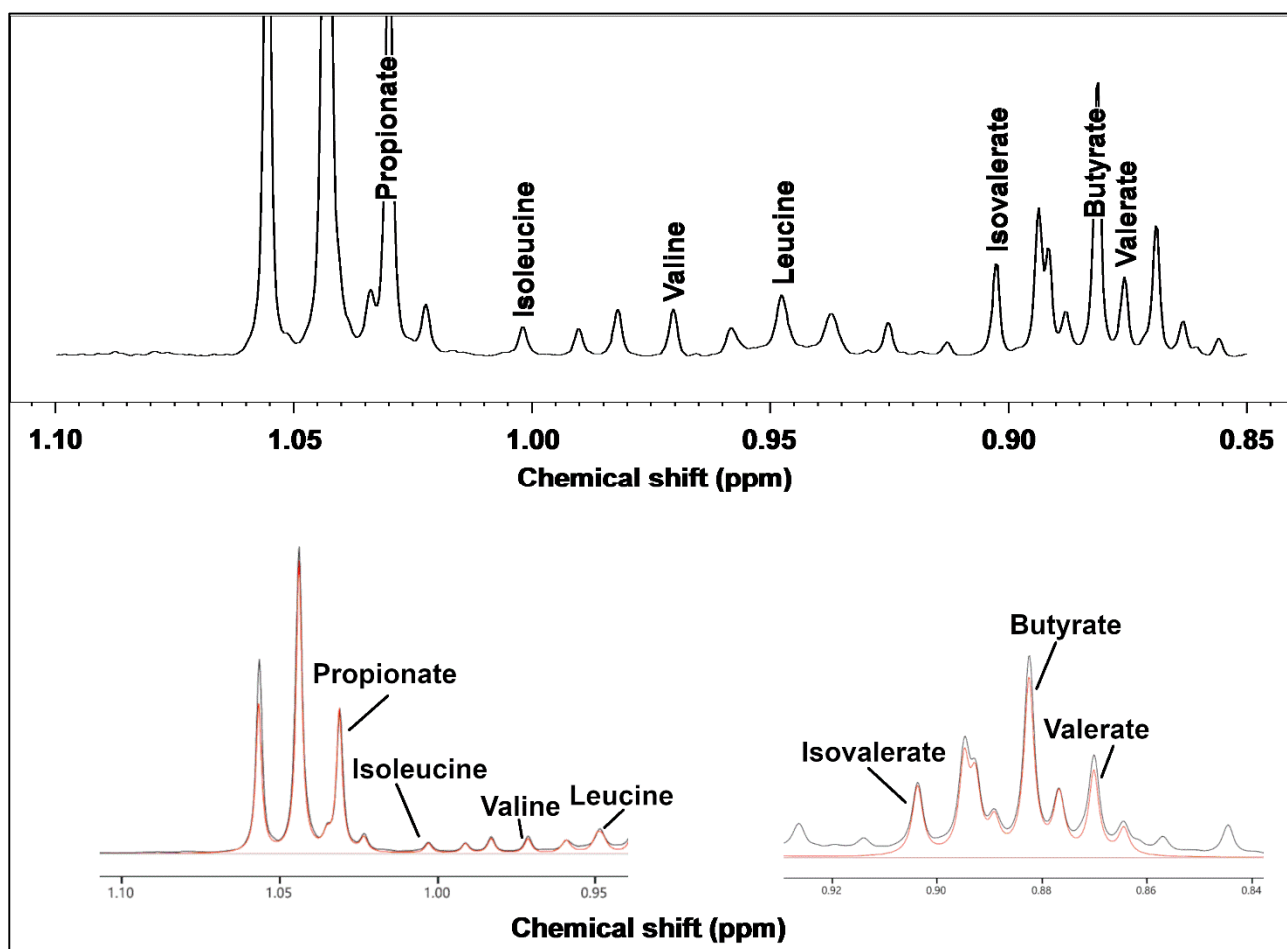
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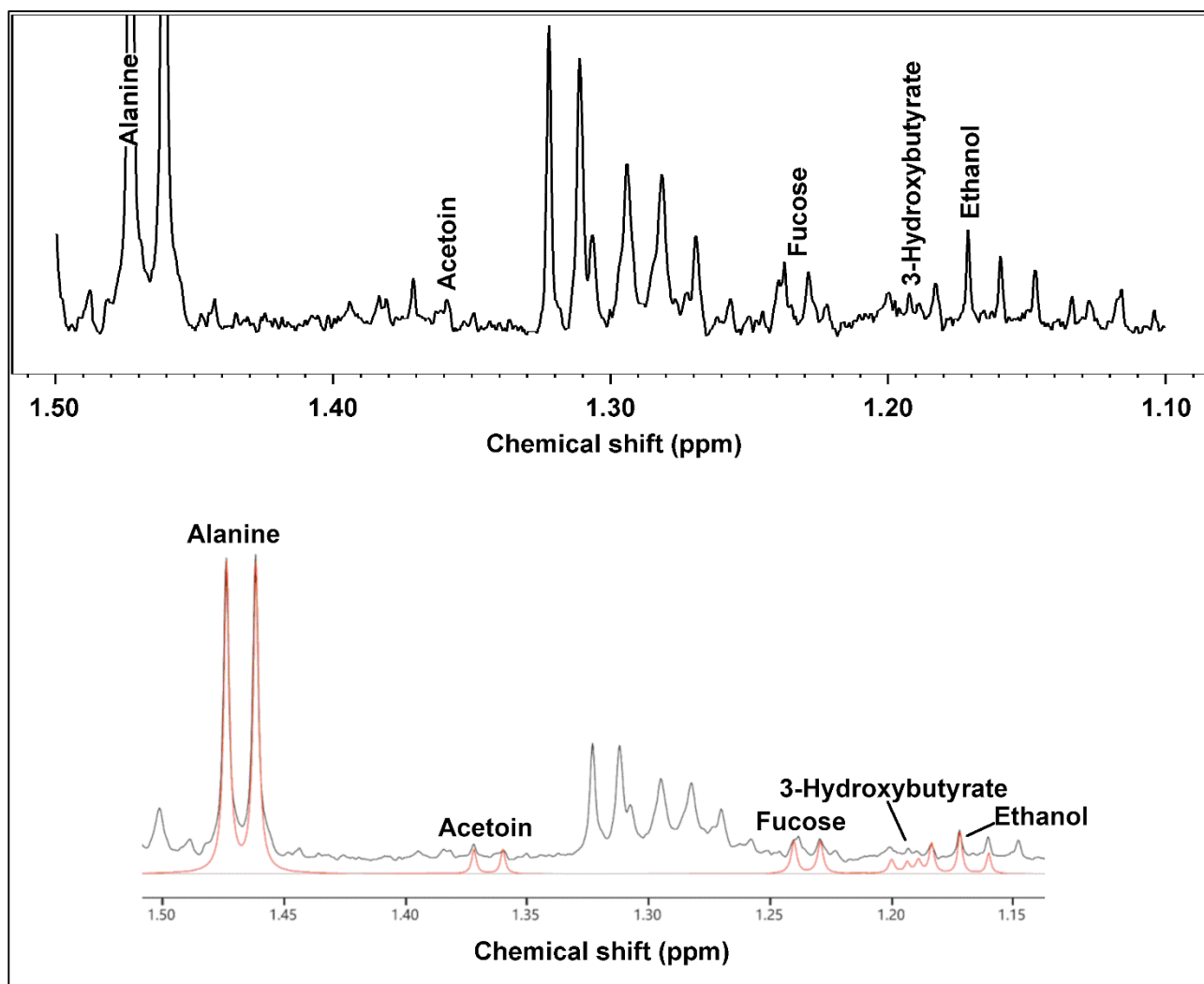


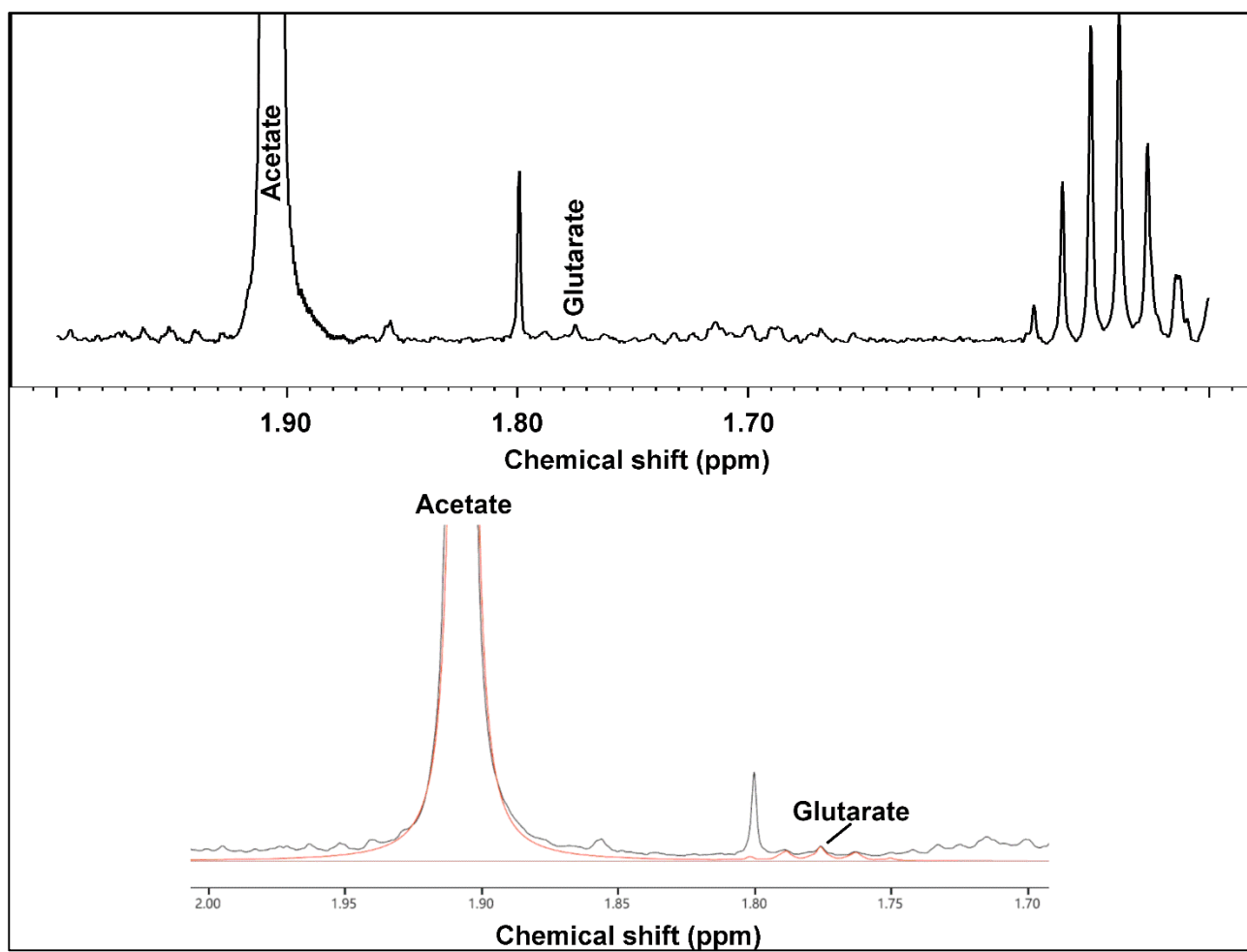


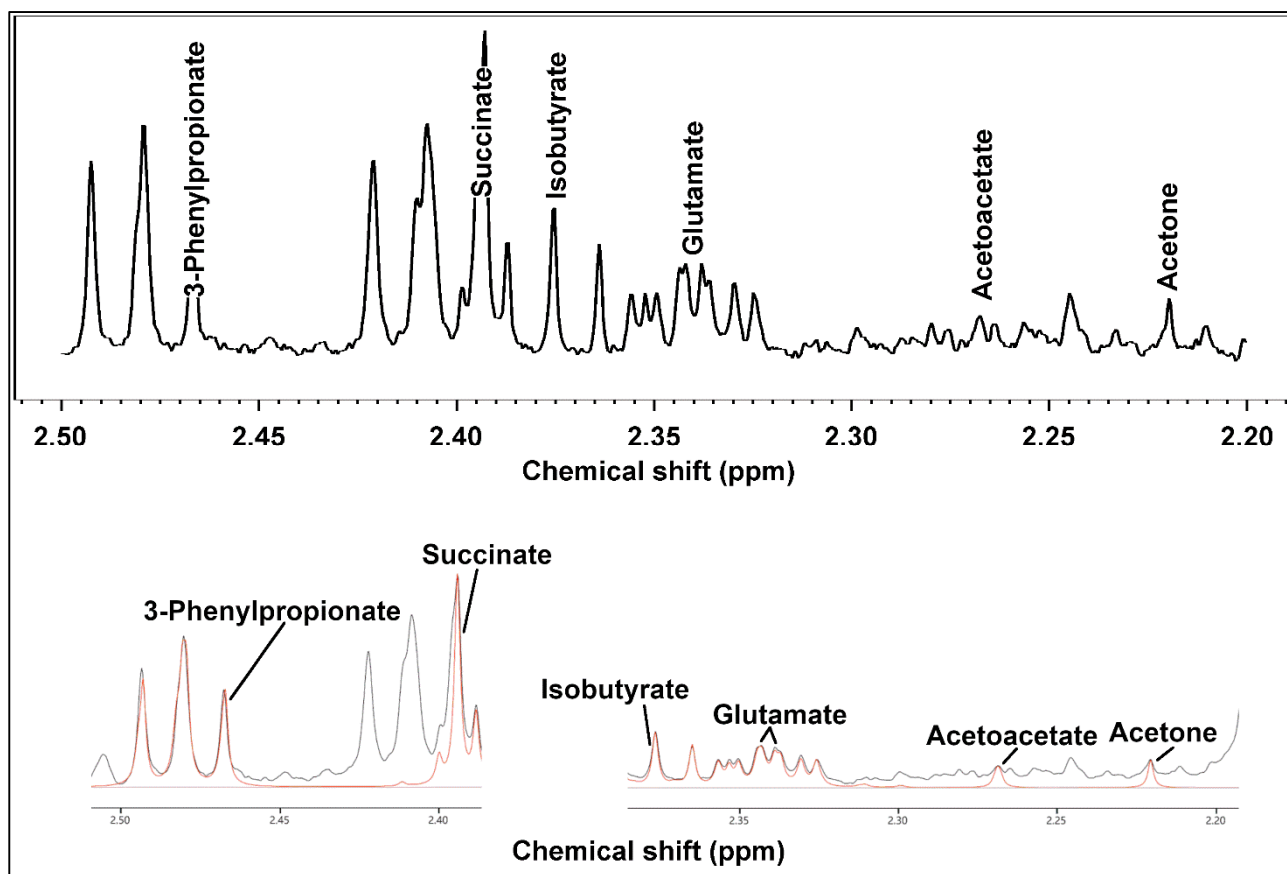


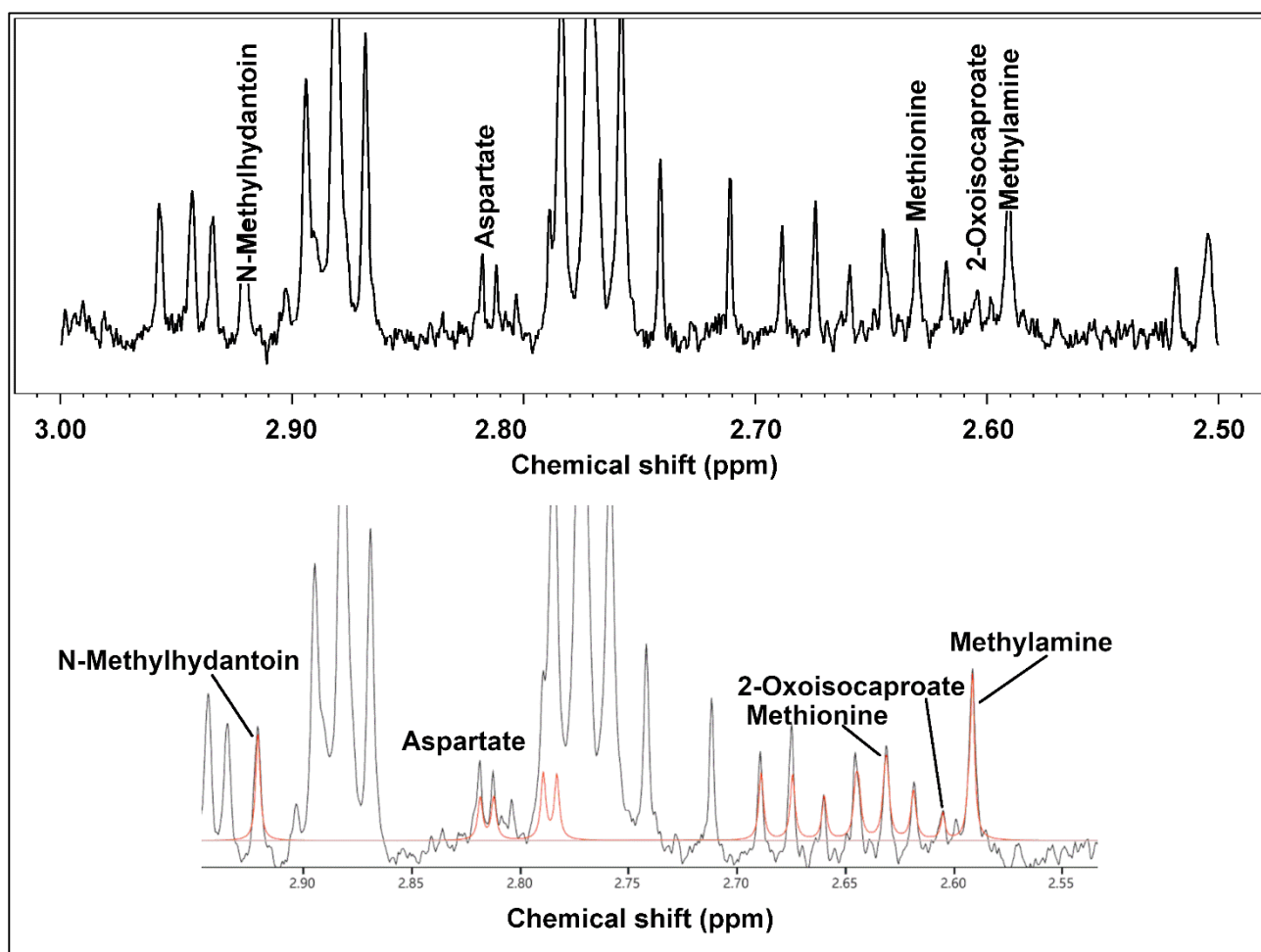
Yak Feces

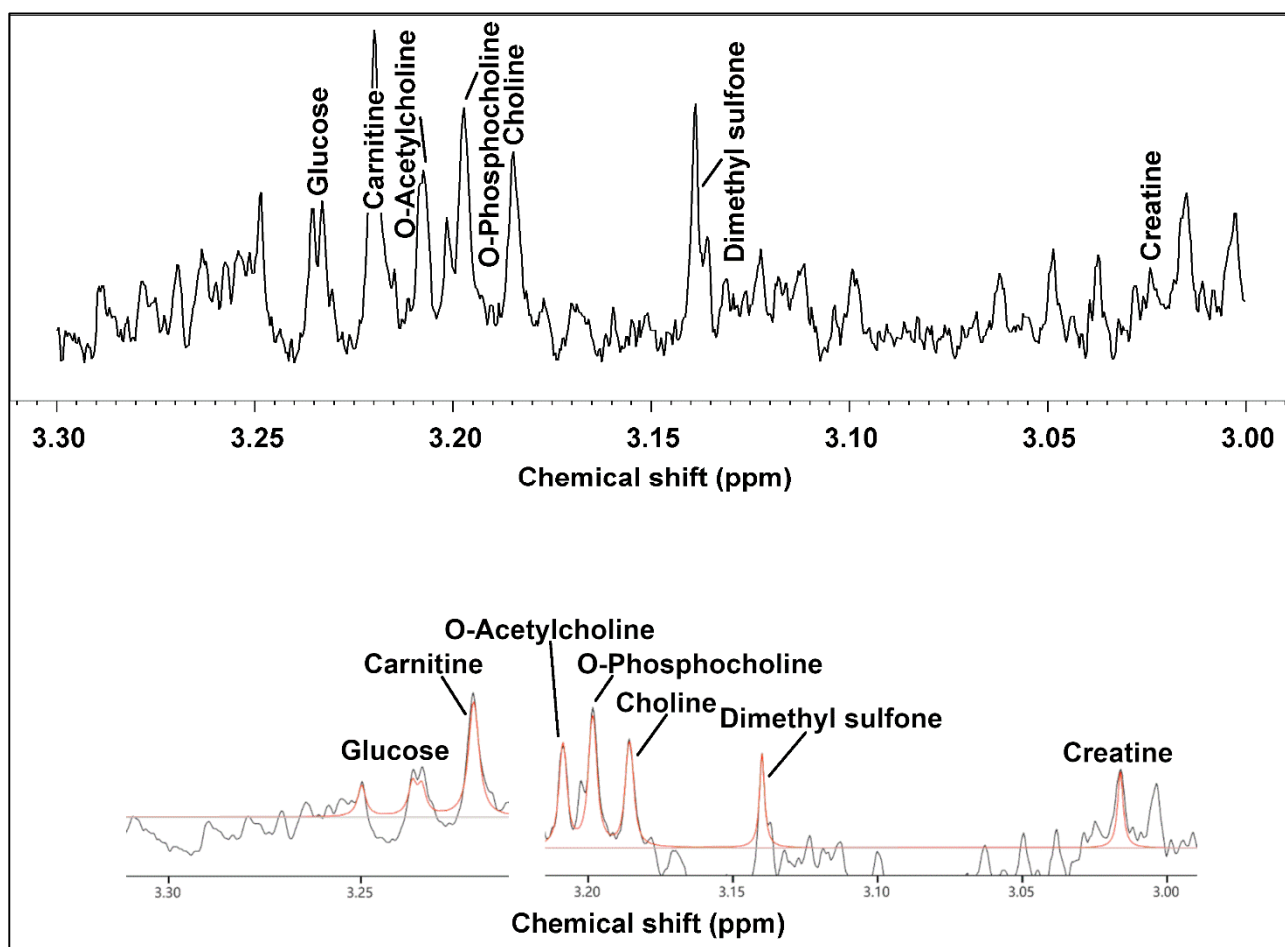


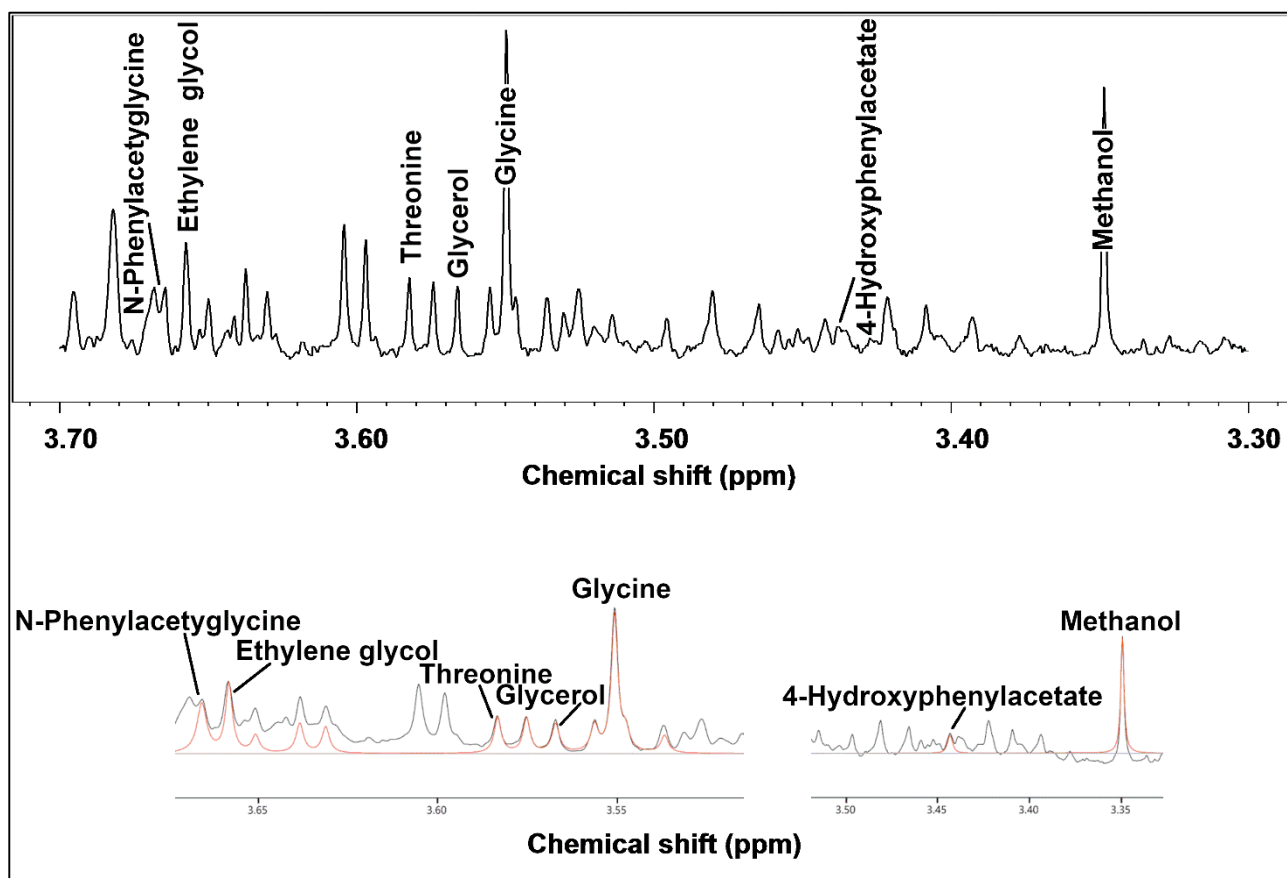


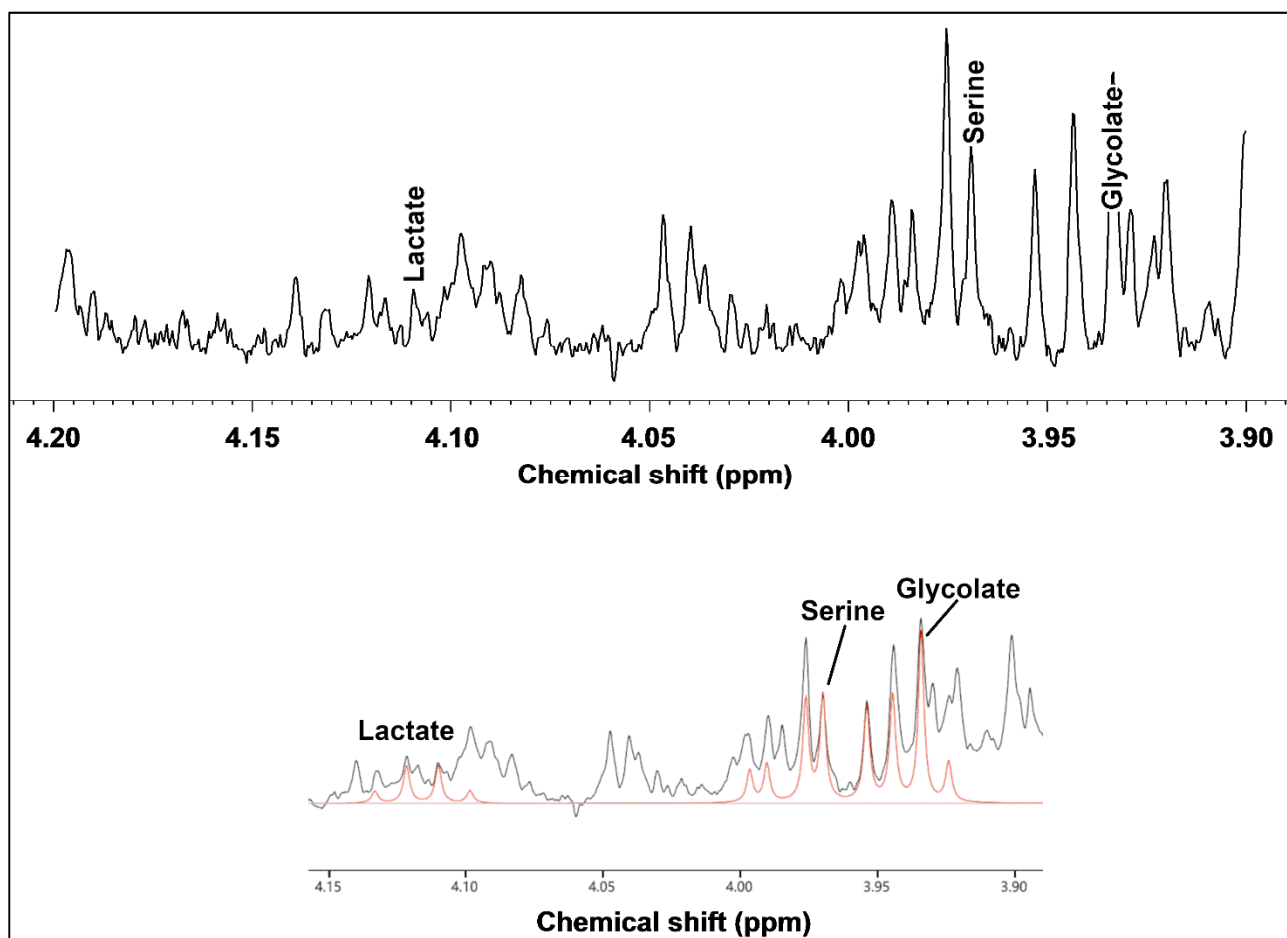


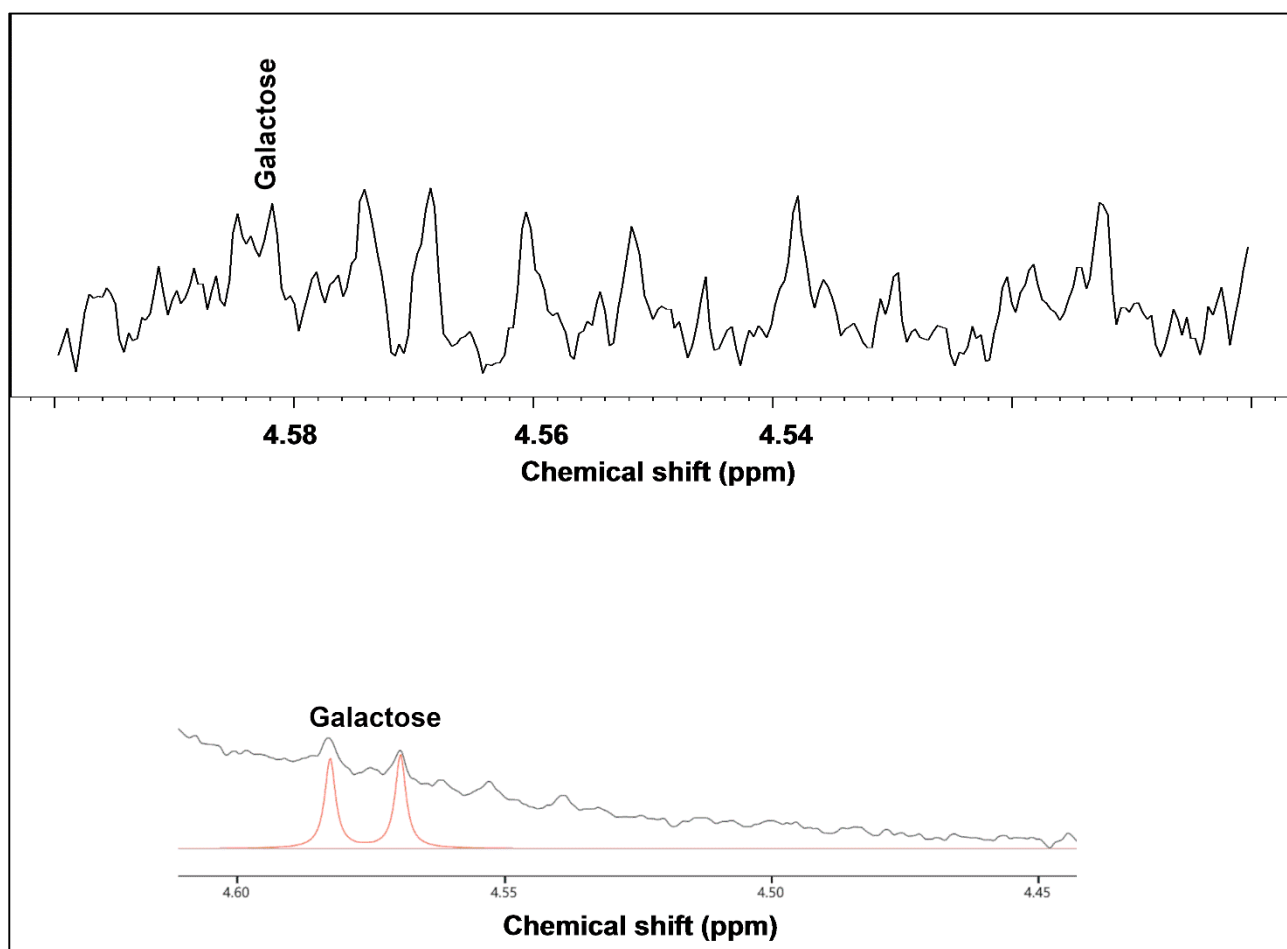


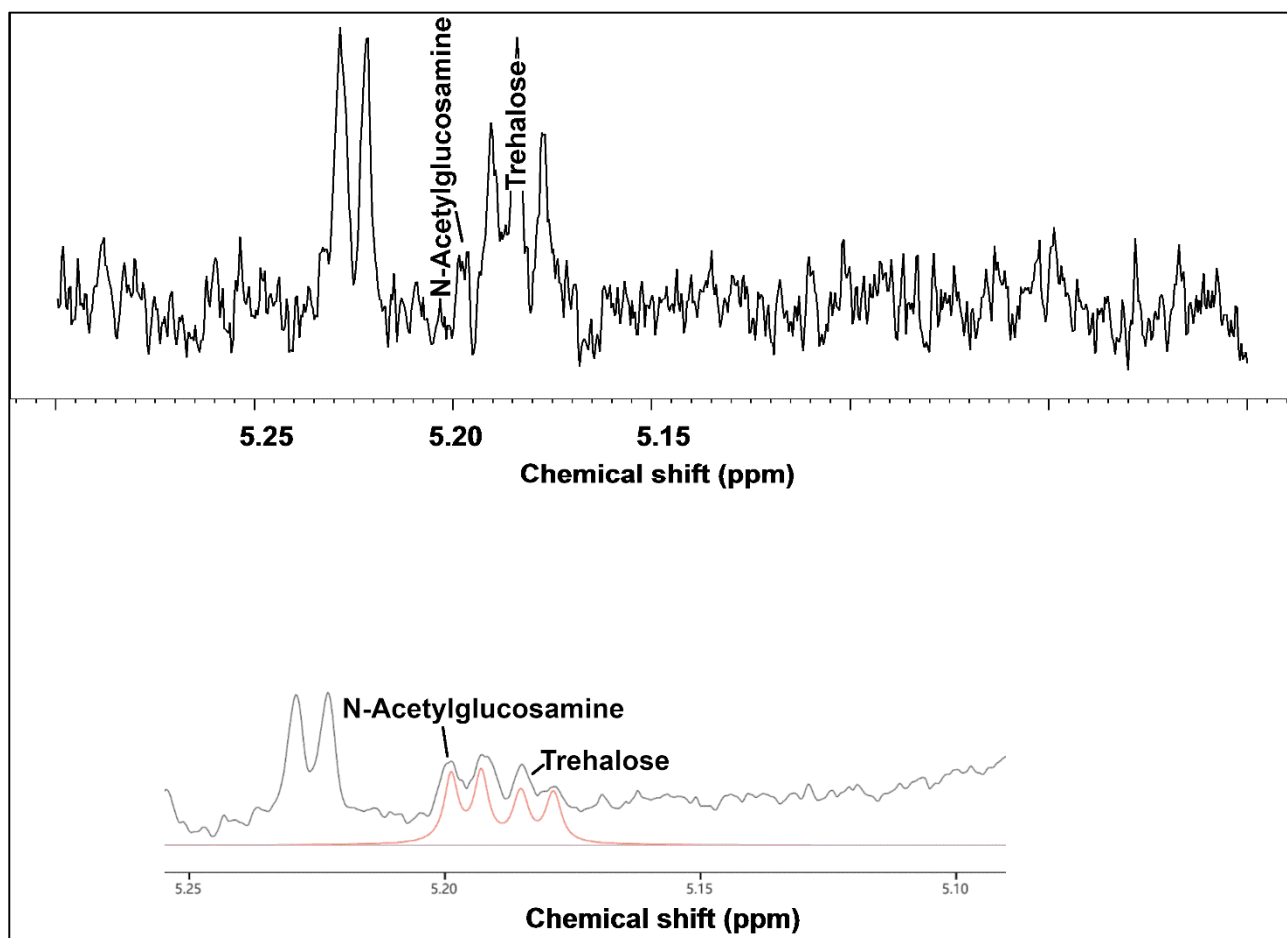


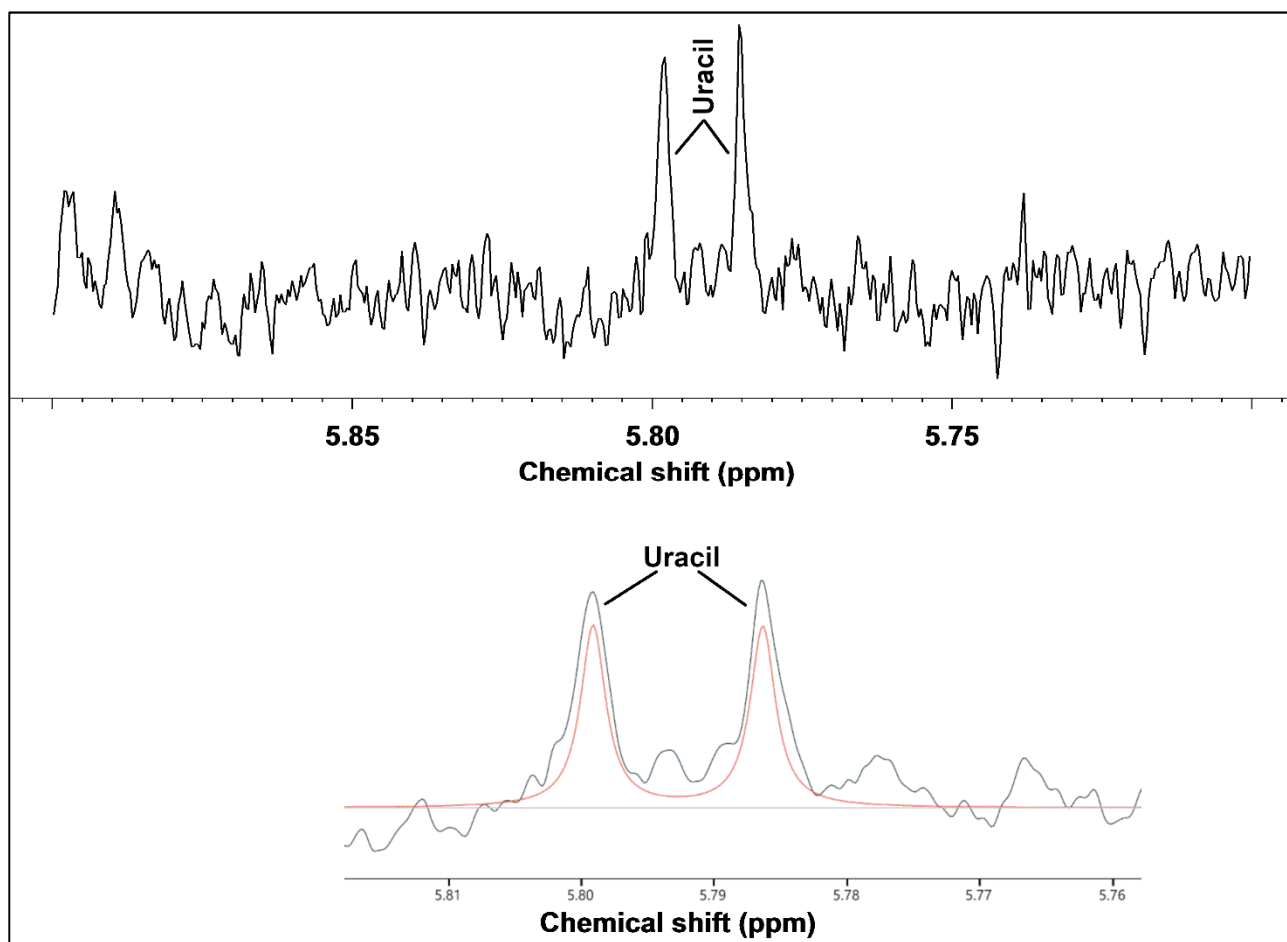


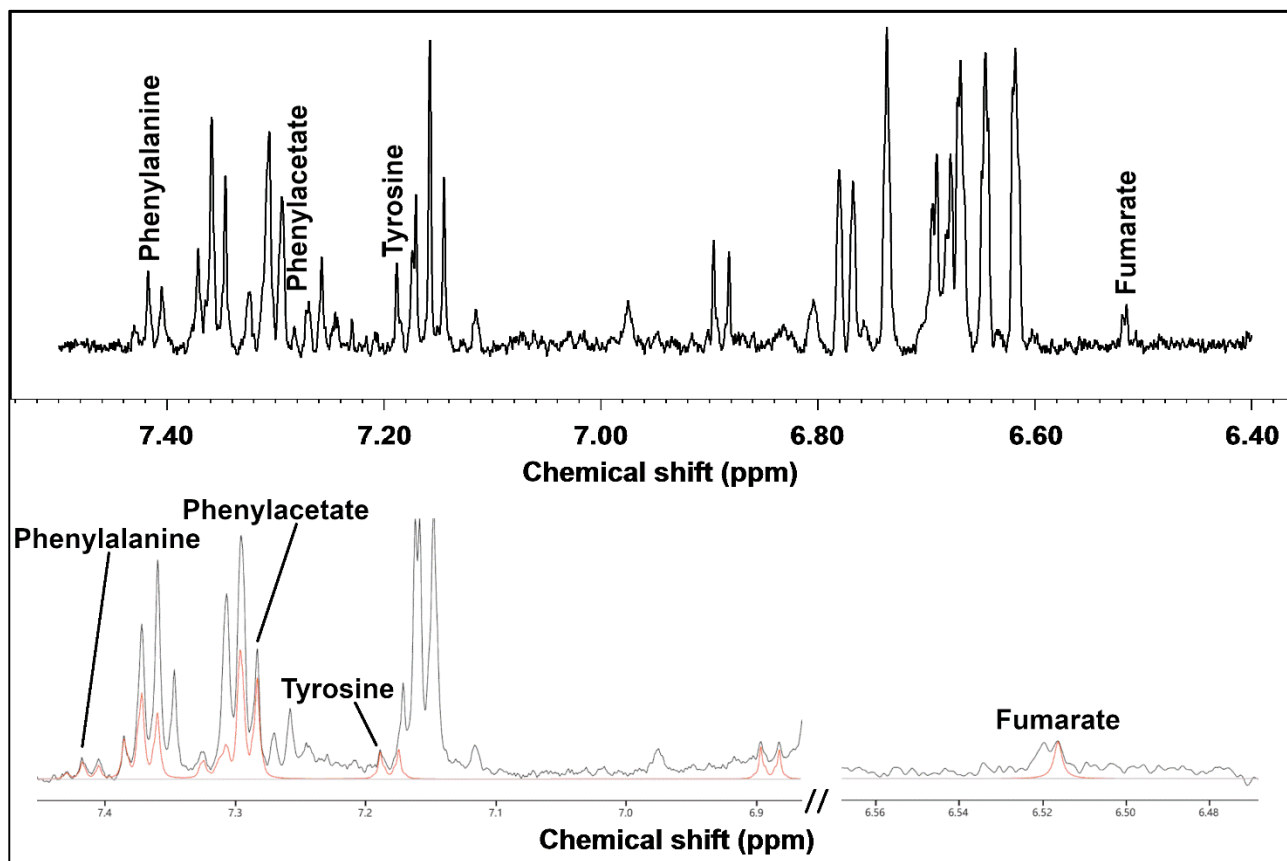


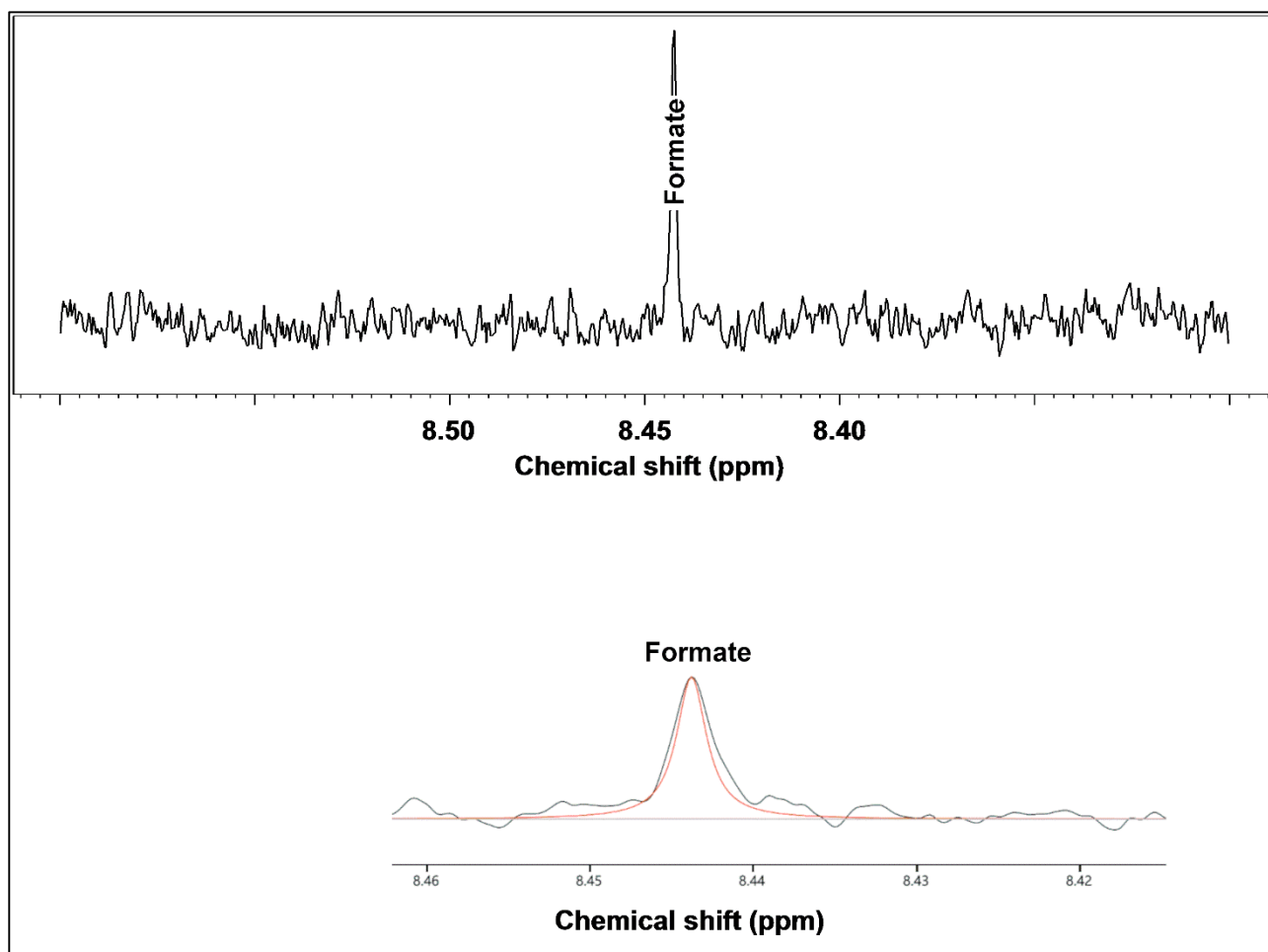




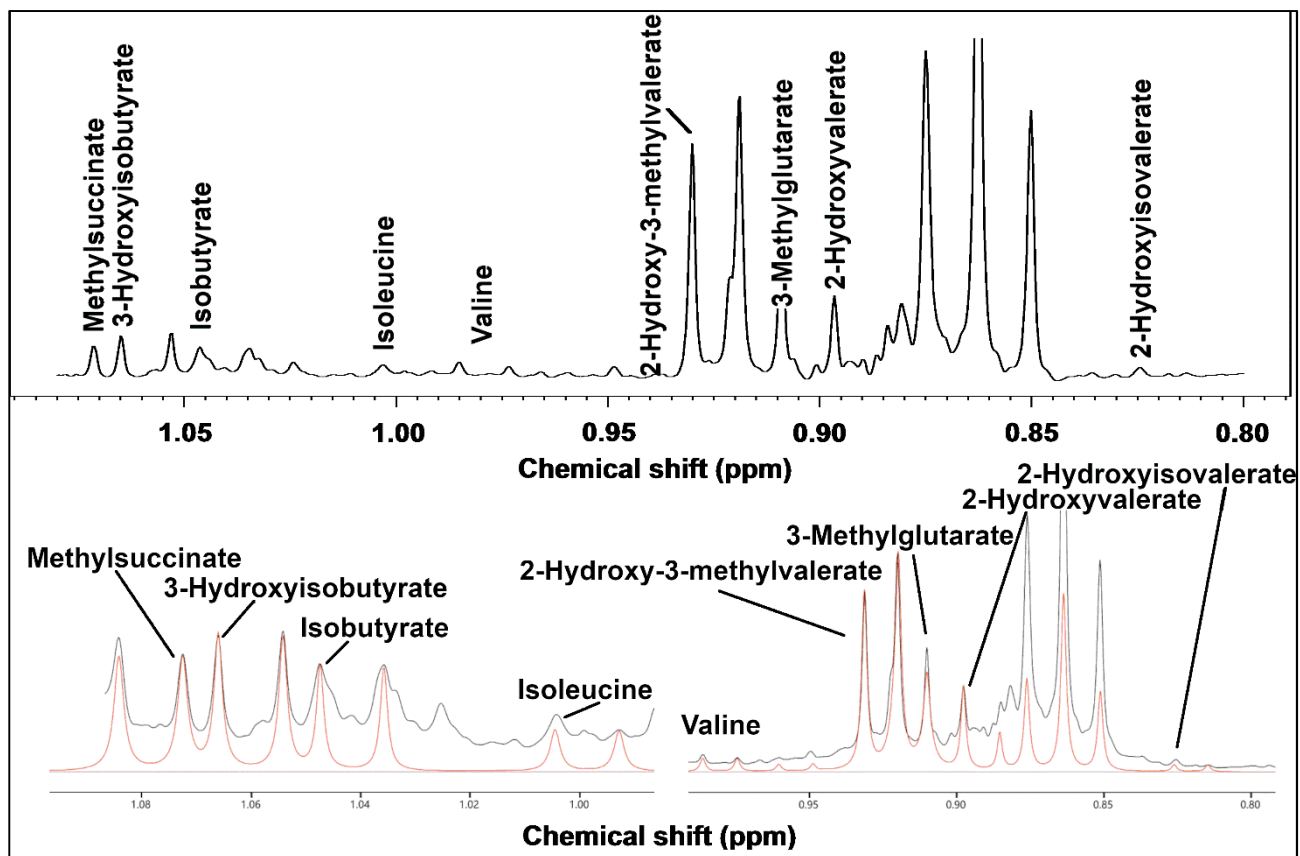




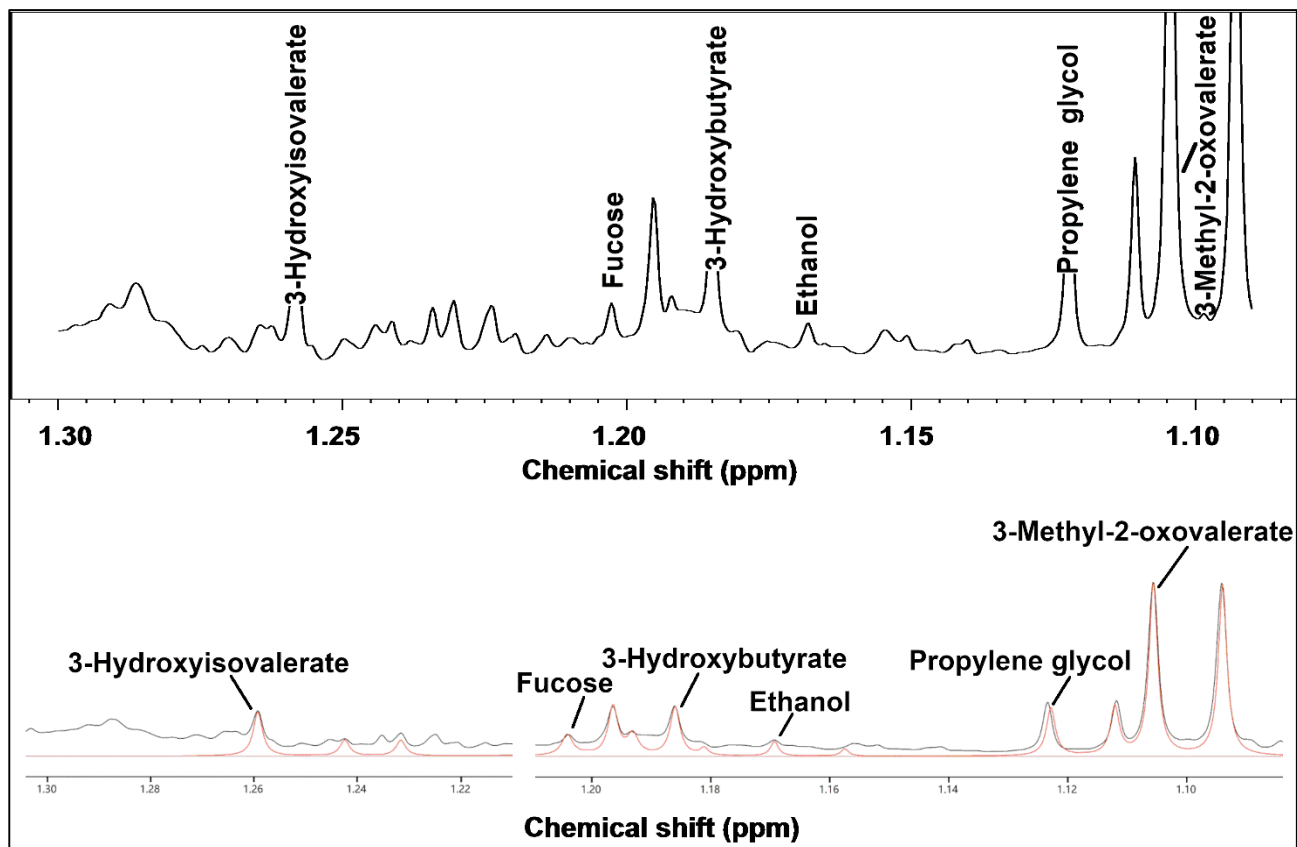




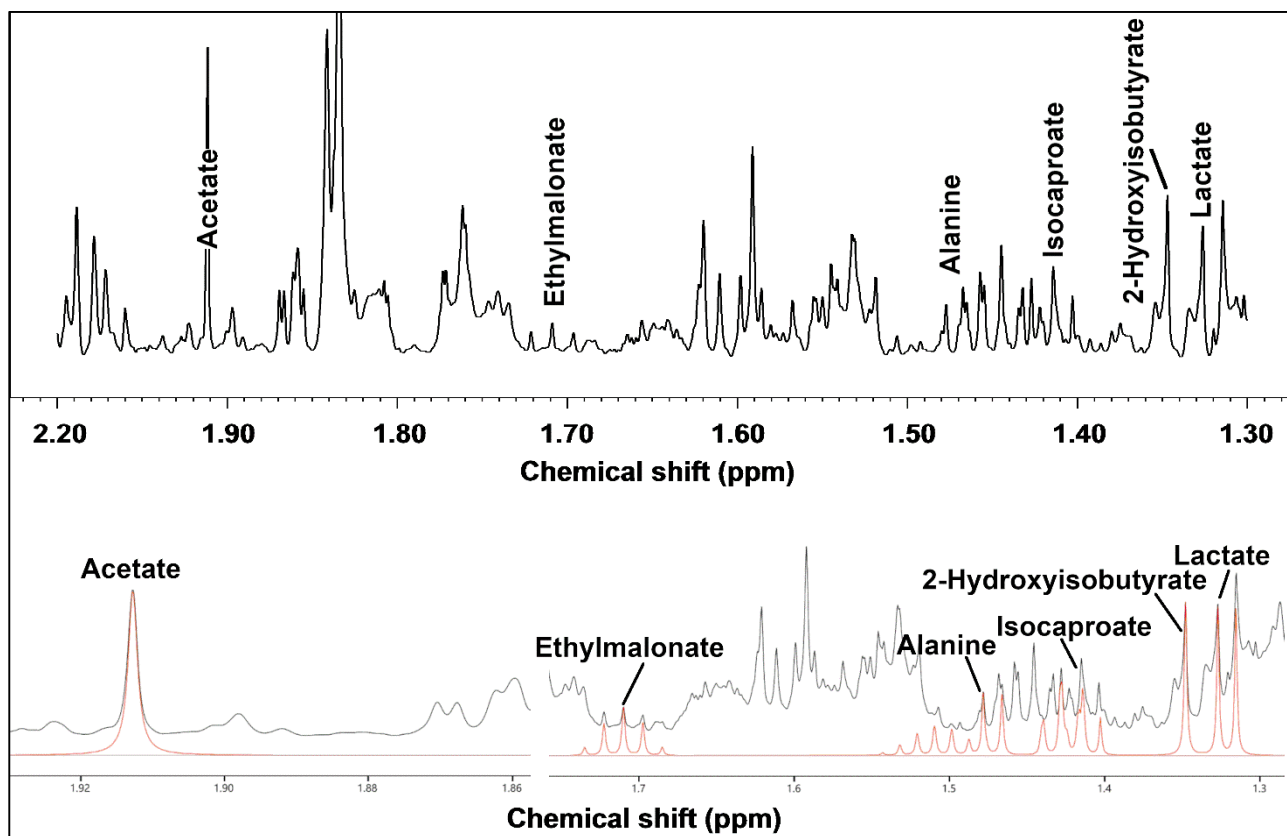
Yak Urine



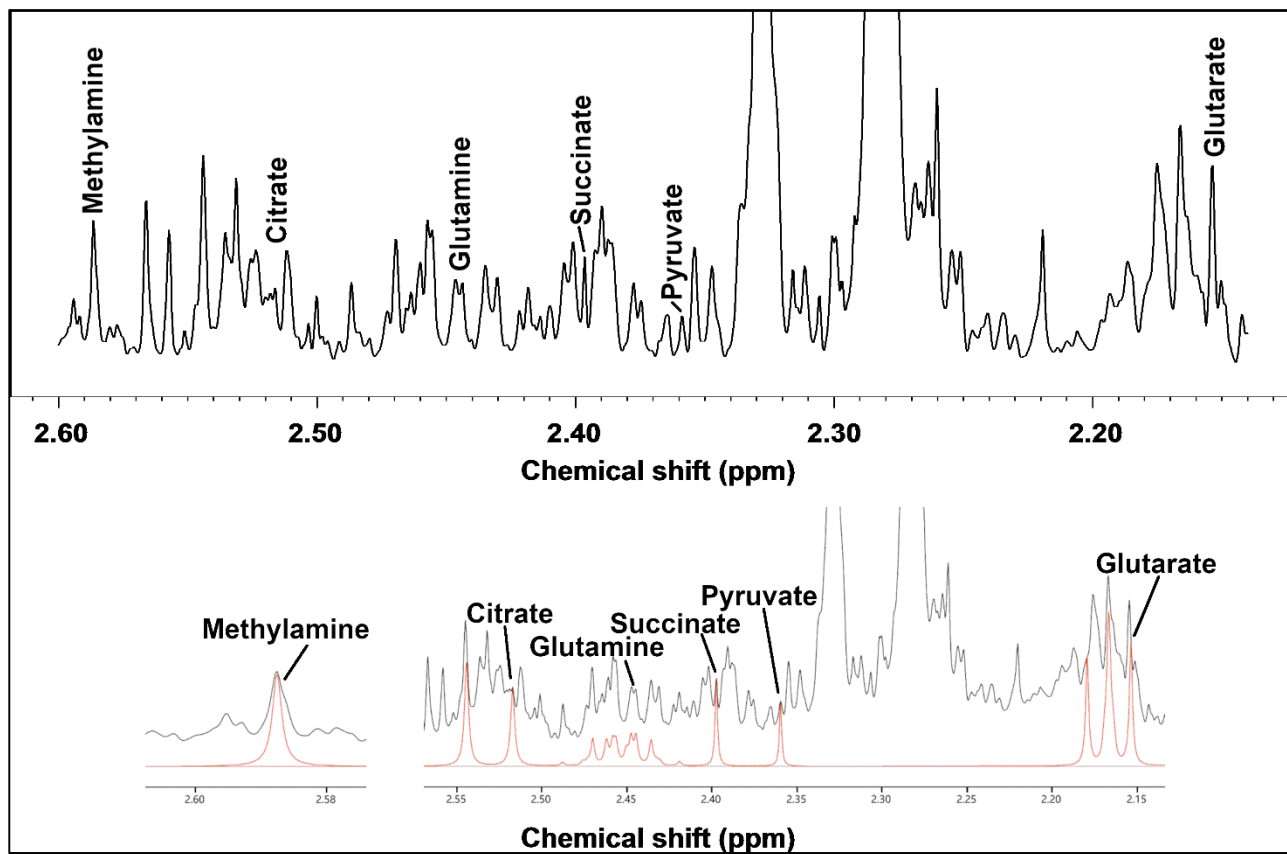
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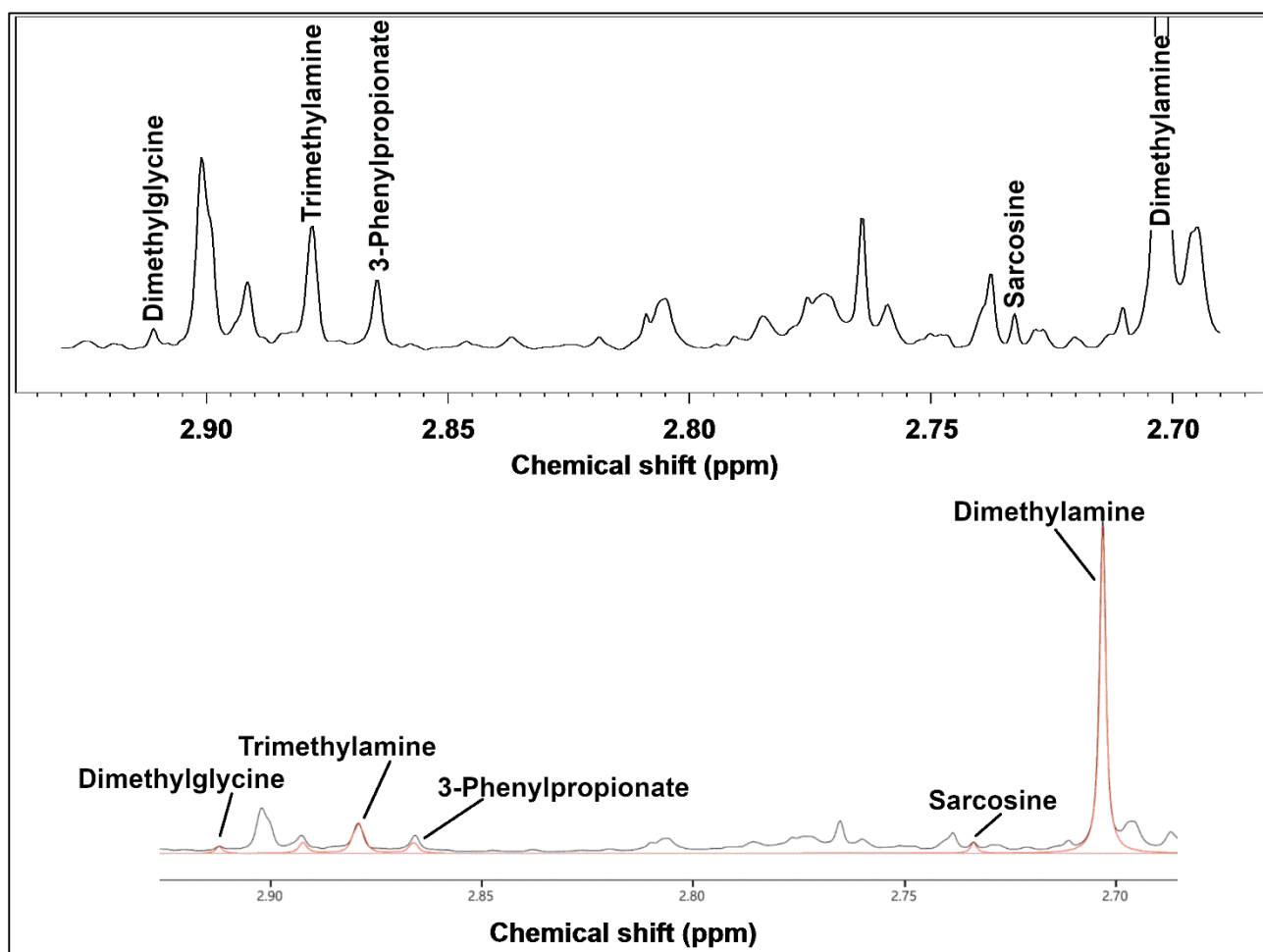
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28

